Wiener Indices of Spiro and Polyphenyl Hexagonal Chains [†]

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Abstract

The Wiener index $W(G)$ of a connected graph G is the sum of distances between all pairs of vertices in G. In this paper, we first give the recurrences or explicit formulae for computing the Wiener indices of spiro and polyphenyl hexagonal chains, which are graphs of a class of unbranched multispiro molecules and polycyclic aromatic hydrocarbons, then we establish a relation between the Wiener indices of a spiro hexagonal chain and its corresponding polyphenyl hexagonal chain, and determine the extremal values and characterize the extremal graphs with respect to the Wiener index among all spiro and polyphenyl hexagonal chains with n hexagons, respectively. An interesting result shows that the average value of the Wiener indices with respect to the set of all such hexagonal chains is exactly the average value of the Wiener indices of three special hexagonal chains, and is just the Wiener index of the meta-chain.

[†]Project supported by the Scientific Research Fund of Hunan Provincial Education Department (09A057) and the Hunan Provincial Natural Science Foundation of China (09JJ6009).

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1 Introduction

All graphs considered in this paper are simple, undirected and connected. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$, respectively. The distance $d_G(u,v)$ between vertices u and v is the number of edges on a shortest path connecting these vertices in G. The distance $W(G,v)$ of a vertex $v \in V(G)$ is the sum of distances between v and all other vertices of G.

The Wiener index [1,2] of a graph G is a graph invariant based on distances. It is defined as the sum of distances between all pairs of vertices in G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) = \frac{1}{2} \sum_{v \in V(G)} W(G,v).$$

Wiener index is the oldest topological index related to molecular branching [3]. A tentative explanation of the relevance of the Wiener index in research of QSPR and QSAR is that it correlates with the van der Waals surface area of the molecule [4]. Until now, the Wiener index has gained much popularity and new results related to it are constantly being reported. For a survey of results and further bibliography on the chemical applications and the mathematical literature of the Wiener index, see [5-8] and the references cited therein.

Spiro compounds are an important class of cycloalkanes in organic chemistry. A spiro union in spiro compounds is a linkage between two rings that consists of a single atom common to both rings and a free spiro union is a linkage that consists of the only direct union between the rings. The common atom is designated as the spiro atom. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc, ring systems. Figure 1(i) illustrates three linear polyspiro alicyclic hydrocarbons. Here, we consider a subclass of unbranched multispiro molecules, in which every ring is a hexagon, and their graphs are called spiro hexagonal chains (or chain hexagonal cacti, or six-membered ring spiro chain [9-11]).

Two or more benzene rings are linked by a cut edges consisting of aromatics called polycyclic aromatic hydrocarbons which is a class of aromatics. A class of compounds in which two and more benzene rings are directly linked by a cut edge known as the biphenyl compounds, and their graphs are called polyphenyl hexagonal chains [12]. Figure 1(ii) illustrates ortho-terphenyl, meta-terphenyl and pera-terphenyl.

Some explicit recurrences for the matching and independence polynomials in the spiro and polyphenyl hexagonal chains were derived in [9], and the spiro and polyphenyl hexagonal chains with the extremal values of the Merrifield-Simmons index and Hosoya index were determined in [11,12]. The extremal energies of the spiro and polyphenyl hexagonal chains were found in [10].

In this paper, we will first give the recurrences or explicit formulae for computing the Wiener indices of spiro and polyphenyl hexagonal chains, and then establish a relation between a spiro hexagonal chain and its corresponding polyphenyl hexagonal chain and determine the extremal values and characterize the extremal graphs with respect to the Wiener index among all spiro hexagonal chains and polyphenyl hexagonal chains with n hexagons. Also, we will discuss the average value of the Wiener indices with respect to the set of all such hexagonal chains, and find an interesting result which shows that the average value is exactly the average value of three special hexagonal chains, and is just the Wiener index of the meta-chain.

2 Wiener index of spiro hexagonal chains

A hexagonal cactus is a connected graph in which every block is a hexagon. A vertex shared by two or more hexagons is called a cut-vertex. If each hexagon of a hexagonal cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two hexagons, then G is called a spiro hexagonal chain. The number of hexagons in G is called the length of G. An example of a spiro hexagonal chain is shown in Figure 2(i).

Obviously, a spiro hexagonal chain of length n has $5n + 1$ vertices and $6n$ edges. Furthermore, any spiro hexagonal chain of length greater than one has exactly two hexagons with only one cut-vertex. Such hexagons are called terminal hexagons. Any remaining hexagons are called internal hexagons.

Let $G_n = H_0H_1 \cdots H_{n-1}$ be a spiro hexagonal chain of length $n(n \geq 3)$. H_k is the $(k + 1)$-th hexagon of G_n, c_k is the common cut-vertex of H_{k-1} and H_k, $k = 1, 2, \cdots, n - 1$. Then, the sequence $(c_2, c_3, \cdots, c_{n-1})$ of length $n - 2$ is called the cut-vertex sequence of G_n. Obviously, G_n is determined completely by its cut-vertex sequence. A vertex v of H_k is said to be ortho-, meta- and para-vertex of H_k if the

distance between v and c_k is 1, 2 and 3, denoted by o_k, m_k and p_k, respectively. Examples of ortho-, meta-, and para-vertices are shown in Figure 3(ii). Except the first hexagon, any hexagon in a spiro hexagonal chain has two ortho-vertices, two meta-vertices and one para-vertex.

A spiro hexagonal chain G_n is a spiro ortho-chain if $c_k = o_{k-1}$ for $2 \leq k \leq n-1$, i.e., its cut-vertex sequence is $(o_1, o_2, \cdots, o_{n-2})$. The spiro meta-chain and spiro para-chain are defined in a completely analogous manner. The spiro ortho-, meta- and para-chain of length n is denoted by O_n, M_n and P_n, respectively. Examples of spiro ortho-, meta-, and para-chains are shown in Figure 4.

In the following, we first give a recurrence for computing the Wiener indices of spiro hexagonal chains, and then derive a formula for computing the Wiener indices of spiro hexagonal chains.

Let $G_n = H_0 H_1 \cdots H_{n-1}$ be a spiro hexagonal chain with n hexagons as shown in Figure 3(i). $G_{n-1} = H_0 H_1 \cdots H_{n-2}$ and $c_{n-1}, o_{n-1}, m_{n-1}, p_{n-1}$ are the cut-, ortho-, meta-, and para-vertex in H_{n-1}, respectively. Then

$$\begin{aligned} W(G_n, o_{n-1}) &= \sum_{v \in G_n} d(v, o_{n-1}) = \sum_{v \in G_{n-1}} (d(v, c_{n-1}) + 1) + 8 \\ &= W(G_{n-1}, c_{n-1}) + 5(n-1) + 9; \\ W(G_n, m_{n-1}) &= \sum_{v \in G_n} d(v, m_{n-1}) = \sum_{v \in G_{n-1}} (d(v, c_{n-1}) + 2) + 7 \\ &= W(G_{n-1}, c_{n-1}) + 10(n-1) + 9; \\ W(G_n, p_{n-1}) &= \sum_{v \in G_n} d(v, p_{n-1}) = \sum_{v \in G_{n-1}} (d(v, c_{n-1}) + 3) + 6 \\ &= W(G_{n-1}, c_{n-1}) + 15(n-1) + 9. \end{aligned}$$

So, we have

$$W(G_n, c_n) = W(G_{n-1}, c_{n-1}) + f(c_n) \tag{1}$$

where

$$f(c_n) = \begin{cases} 5(n-1) + 9, & c_n \ is \ o_{n-1}; \\ 10(n-1) + 9, & c_n \ is \ m_{n-1}; \\ 15(n-1) + 9, & c_n \ is \ p_{n-1}. \end{cases}$$

Let v_1, v_2, v_3, v_4, v_5 be the vertices of H_{n-1} different from c_{n-1}. By the definition

of Wiener index,

$$\begin{aligned} W(G_n) &= W(G_{n-1}) + \sum_{i=1}^{5} \sum_{v\in G_{n-1}} d(v, v_i) + \sum_{1\le i<j\le 5} d(v_i, v_j) \\ &= W(G_{n-1}) + \sum_{v\in G_{n-1}} (5d(v, c_{n-1}) + 9) + 18 \\ &= W(G_{n-1}) + 5W(G_{n-1}, c_{n-1}) + 45n - 18. \end{aligned}$$

i.e.,

$$W(G_n) = W(G_{n-1}) + 5W(G_{n-1}, c_{n-1}) + 45n - 18. \tag{2}$$

Combining equations (1) and (2), we can get the following recurrence for computing the Wiener indices of spiro hexagonal chains.

Theorem 2.1. Let $G_n = H_0H_1 \cdots H_{n-1}$ be a spiro hexagonal chain of length n, c_{n-1} the cut-vertex of H_{n-1}. Then

$$\begin{cases} W(G_n) = W(G_{n-1}) + 5W(G_{n-1}, c_{n-1}) + 45n - 18, \\ W(G_n, c_n) = W(G_{n-1}, c_{n-1}) + f(c_n), \\ W(G_1) = 27, \\ W(G_1, c_1) = f(c_1) = 9, \end{cases}$$

and

$$f(c_n) = \begin{cases} 5(n-1) + 9, & c_n \ is \ o_{n-1}; \\ 10(n-1) + 9, & c_n \ is \ m_{n-1}; \\ 15(n-1) + 9, & c_n \ is \ p_{n-1}. \end{cases}$$

Using the recurrence for computing the Wiener indices of spiro hexagonal chains, we have

$$\begin{aligned} W(G_n) &= W(G_{n-1}) + 5W(G_{n-1}, c_{n-1}) + 45n - 18 \\ &= W(G_1) + 5\sum_{k=1}^{n-1} W(G_{n-k}, c_{n-k}) + 45\sum_{k=1}^{n-1}(n-k+1) - 18(n-1) \\ &= 27 + 5\sum_{k=1}^{n-1} W(G_k, c_k) + \tfrac{45}{2}(n+2)(n-1) - 18(n-1) \\ &= 5\sum_{k=1}^{n-1} W(G_k, c_k) + \tfrac{45}{2}n^2 + \tfrac{9}{2}n \end{aligned}$$

i.e.,

$$W(G_n) = 5\sum_{k=1}^{n-1} W(G_k, c_k) + \frac{45}{2}n^2 + \frac{9}{2}n. \tag{3}$$

And,

$$\begin{aligned} W(G_k, c_k) &= W(G_{k-1}, c_{k-1}) + f(c_k) \\ &= W(G_1, c_1) + f(c_2) + \cdots + f(c_k) \\ &= f(c_1) + f(c_2) + \cdots + f(c_k), \end{aligned}$$

i.e.,

$$W(G_k, c_k) = \sum_{i=1}^{k} f(c_i). \tag{4}$$

Combining equations (3) and (4), we can obtain the following formula for computing the Wiener indices of spiro hexagonal chains.

Theorem 2.2. Let $G_n = H_0H_1 \cdots H_{n-1}$ be a spiro hexagonal chain with n hexagons. c_k is the common cut-vertex of H_{k-1} and H_k, $1 \leq k \leq n-1$. Then

$$\begin{aligned} W(G_n) &= 5\sum_{k=1}^{n-1}\sum_{i=1}^{k} f(c_i) + \tfrac{45}{2}n^2 + \tfrac{9}{2}n \\ &= 5\sum_{k=1}^{n-1}(n-k)f(c_k) + \tfrac{45}{2}n^2 + \tfrac{9}{2}n \end{aligned}$$

where

$$f(c_k) = \begin{cases} 5(k-1)+9, & c_k \ is \ o_{k-1}; \\ 10(k-1)+9, & c_k \ is \ m_{k-1}; \\ 15(k-1)+9, & c_k \ is \ p_{k-1}. \end{cases} \tag{5}$$

and $f(c_1) = 9$.

In the spiro orth-chain O_n, the spiro meta-chain M_n and the spiro para-chain P_n, c_k is o_{k-1}, m_{k-1} and p_{k-1}, respectively. Then

$W(O_n) = 5\sum_{k=1}^{n-1}(n-k)(5(k-1)+9) + \frac{45}{2}n^2 + \frac{9}{2}n = \frac{25}{6}n^3 + \frac{65}{2}n^2 - \frac{29}{3}n;$

$W(M_n) = 5\sum_{k=1}^{n-1}(n-k)(10(k-1)+9) + \frac{45}{2}n^2 + \frac{9}{2}n = \frac{25}{3}n^3 + 20n^2 - \frac{4}{3}n;$

$W(P_n) = 5\sum_{k=1}^{n-1}(n-k)(15(k-1)+9) + \frac{45}{2}n^2 + \frac{9}{2}n = \frac{25}{2}n^3 + \frac{15}{2}n^2 + 7n.$

Corollary 2.3. The Wiener indices of the spiro orth-chain O_n, the spiro meta-chain M_n and the spiro para-chain P_n are

$$W(O_n) = \frac{25}{6}n^3 + \frac{65}{2}n^2 - \frac{29}{3}n;$$

$$W(M_n) = \frac{25}{3}n^3 + 20n^2 - \frac{4}{3}n;$$

$$W(P_n) = \frac{25}{2}n^3 + \frac{15}{2}n^2 + 7n.$$

In the following, we consider the extremal problems of Wiener indices among all spiro hexagonal chains with n hexagons.

Let $G_n = H_0H_1 \cdots H_{n-1}$ be a spiro hexagonal chain with n hexagons, c_k is the common cut-vertex of H_{k-1} and H_k, $1 \leq k \leq n-1$. From Theorem 2.2 and $5k+9 <$

$10k+9 < 15k+9$, i.e., $f(o_k) < f(m_k) < f(p_k)$ for $k > 1$, it is easily showed that O_n is the unique spiro hexagonal chain with the minimum Wiener index, and the unique spiro hexagonal chain with the second minimal Wiener index is the spiro hexagonal chain G_n with the cut-vertex sequence $(c_2, \cdots, c_{n-2}, c_{n-1}) = (o_1, \cdots, o_{n-3}, m_{n-2})$. In order to find the third minimal value, we only need to compare $2f(m_{n-3}) + f(o_{n-2})$ with $2f(o_{n-3}) + f(p_{n-2})$ from Theorem 2.2. Since $2f(m_{n-3}) + f(o_{n-2}) < 2f(o_{n-3}) + f(p_{n-2})$, the unique spiro hexagonal chain with the third minimal Wiener index is the spiro hexagonal chain G_n with $(c_2, \cdots, c_{n-3}, c_{n-2}, c_{n-1}) = (o_1, \cdots, o_{n-4}, m_{n-3}, o_{n-2})$.

Theorem 2.4. Among all spiro hexagonal chains with $n(n \geq 4)$ hexagons, (i) the unique spiro hexagonal chain with the minimum Wiener index is O_n; (ii) the unique spiro hexagonal chain with the second minimal Wiener index is the spiro hexagonal chain G_n with the cut-vertex sequence $(c_2, \cdots, c_{n-1}) = (o_1, \cdots, o_{n-3}, m_{n-2})$; (iii) the unique spiro hexagonal chain with the third minimal Wiener index is the spiro hexagonal chain G_n with $(c_2, \cdots, c_{n-1}) = (o_1, \cdots, o_{n-4}, m_{n-3}, o_{n-2})$.

Analogously, the following results can be obtained. We omit their proof and leave it for the reader.

Theorem 2.5. Among all spiro hexagonal chains with $n(n \geq 4)$ hexagons, (i) the unique spiro hexagonal chain with the maximum Wiener index is P_n; (ii) the unique spiro hexagonal chain with the second maximal Wiener index is the spiro hexagonal chain G_n with the cut-vertex sequence $(c_2, \cdots, c_{n-2}, c_{n-1}) = (p_1, \cdots, p_{n-3}, m_{n-2})$; (iii) the unique spiro hexagonal chain with the third maximal Wiener index is the spiro hexagonal chain G_n with $(c_2, \cdots, c_{n-3}, c_{n-2}, c_{n-1}) = (p_1, \cdots, p_{n-4}, m_{n-3}, p_{n-2})$.

3 Wiener index of polyphenyl hexagonal chains

In this section, we will give a recurrence for computing the Wiener indices of polyphenyl hexagonal chains, and then derive a formula for computing the Wiener indices of polyphenyl hexagonal chains.

Let G be a cactus graph in which each block is either an edge or a hexagon. G is called a polyphenyl hexagonal chain if each hexagon of G has at most two cut-vertices,

and each cut-vertex is shared by exactly one hexagon and one cut-edge. The number of hexagons in G is called the length of G. An example of a polyphenyl hexagonal chain is shown in Figure 2(ii).

Obviously, a polyphenyl hexagonal chain of length n has $6n$ vertices and $7n-1$ edges. Furthermore, any polyphenyl hexagonal chain of length greater than one has exactly two hexagons with only one cut-vertex. Such hexagons are called terminal hexagons. Any remaining hexagons are called internal hexagons.

Note that any polyphenyl hexagonal chain $\overline{G}_n = \overline{H}_0\overline{H}_1\cdots\overline{H}_{n-1}$ of length $n (n \geq 2)$ can be obtained from the polyphenyl hexagonal chain $\overline{G}_{n-1} = \overline{H}_0\overline{H}_1\cdots\overline{H}_{n-2}$ of length $n-1$ by a cut-edge linking a vertex c_{n-1} in the hexagon $\overline{H}_{n-1}$ to a non cut-vertex u in the terminal hexagon $\overline{H}_{n-2}$ of $\overline{G}_{n-1}$, where u is said to be the tail of $\overline{H}_{n-1}$, denoted by t_{n-1}. A vertex v of $\overline{H}_{n-1}$ is said to be ortho-, meta- and para-vertex if the distance between v and c_{n-1} is 1, 2 and 3, denoted by o_{n-1}, m_{n-1} and p_{n-1}, respectively. Examples of tail, ortho-, meta-, and para-vertices are shown in Figure 5.

A polyphenyl hexagonal chain $\overline{G}_n$ is a polyphenyl ortho-chain if $t_k = o_{k-1}$ for $2 \leq k \leq n-1$. The polyphenyl meta-chain and polyphenyl para-chain are defined in a completely analogous manner. The polyphenyl ortho-, meta- and para-chain of length n is denoted by $\overline{O}_n$, $\overline{M}_n$ and $\overline{P}_n$, respectively. Examples of polyphenyl ortho-, meta-, and para-chains are shown in Figure 6.

Let $\overline{G}_n = \overline{H}_0\overline{H}_1\cdots\overline{H}_{n-1}$ be a polyphenyl hexagonal chain with n hexagons. $\overline{G}_{n-1} = \overline{H}_0\overline{H}_1\cdots\overline{H}_{n-2}$ and $t_{n-1}, o_{n-1}, m_{n-1}, p_{n-1}$ are the tail-, ortho-, meta-, and para-vertex in $\overline{H}_{n-1}$, respectively. Then

$$\begin{aligned}
W(\overline{G}_n, o_{n-1}) &= \sum_{v\in\overline{G}_n} d(v, o_{n-1}) = \sum_{v\in\overline{G}_{n-1}} (d(v, t_{n-1}) + 2) + 9 \\
&= W(\overline{G}_{n-1}, t_{n-1}) + 12(n-1) + 9; \\
W(\overline{G}_n, m_{n-1}) &= \sum_{v\in\overline{G}_n} d(v, m_{n-1}) = \sum_{v\in\overline{G}_{n-1}} (d(v, t_{n-1}) + 3) + 9 \\
&= W(\overline{G}_{n-1}, t_{n-1}) + 18(n-1) + 9; \\
W(\overline{G}_n, p_{n-1}) &= \sum_{v\in\overline{G}_n} d(v, p_{n-1}) = \sum_{v\in\overline{G}_{n-1}} (d(v, t_{n-1}) + 4) + 9 \\
&= W(\overline{G}_{n-1}, t_{n-1}) + 24(n-1) + 9.
\end{aligned}$$

So, we have

$$W(\overline{G}_n, t_n) = W(\overline{G}_{n-1}, t_{n-1}) + g(t_n) \tag{6}$$

where

$$g(t_n) = \begin{cases} 12(n-1)+9, & t_n \ is \ o_{n-1}; \\ 18(n-1)+9, & t_n \ is \ m_{n-1}; \\ 24(n-1)+9, & t_n \ is \ p_{n-1}. \end{cases}$$

Let $v_1, v_2, v_3, v_4, v_5, v_6$ be the vertices of $\overline{H}_{n-1}$ different from the tail t_{n-1}. By the definition of Wiener index,

$$\begin{aligned} W(\overline{G}_n) &= W(\overline{G}_{n-1}) + \sum_{i=1}^{6} \sum_{v \in \overline{G}_{n-1}} d(v, v_i) + \sum_{1 \le i < j \le 6} d(v_i, v_j) \\ &= W(\overline{G}_{n-1}) + \sum_{v \in \overline{G}_{n-1}} (6d(v, t_{n-1}) + 15) + 27 \\ &= W(\overline{G}_{n-1}) + 6W(\overline{G}_{n-1}, t_{n-1}) + 90n - 63, \end{aligned}$$

i.e.,

$$W(\overline{G}_n) = W(\overline{G}_{n-1}) + 6W(\overline{G}_{n-1}, t_{n-1}) + 90n - 63. \tag{7}$$

Combining equations (6) and (7), we can get the following recurrence for computing the Wiener indices of polyphenyl hexagonal chains.

Theorem 3.1. Let $\overline{G}_n = \overline{H}_0 \overline{H}_1 \cdots \overline{H}_{n-1}$ be a polyphenyl hexagonal chain with n hexagons, t_{n-1} the tail of $\overline{H}_{n-1}$. Then

$$\begin{cases} W(\overline{G}_n) = W(\overline{G}_{n-1}) + 6W(\overline{G}_{n-1}, t_{n-1}) + 90n - 63, \\ W(\overline{G}_n, t_n) = W(\overline{G}_{n-1}, t_{n-1}) + g(t_n), \\ W(\overline{G}_1) = W(\overline{H}_0) = 27, \\ W(\overline{G}_1, t_1) = g(t_1) = 9, \end{cases}$$

and

$$g(t_n) = \begin{cases} 12(n-1)+9, & t_n \ is \ o_{n-1}; \\ 18(n-1)+9, & t_n \ is \ m_{n-1}; \\ 24(n-1)+9, & t_n \ is \ p_{n-1}. \end{cases}$$

Using the recurrence above, we have

$$\begin{aligned} W(\overline{G}_n) &= W(\overline{G}_{n-1}) + 6W(\overline{G}_{n-1}, t_{n-1}) + 90n - 63 \\ &= W(\overline{G}_1) + 6\sum_{k=1}^{n-1} W(\overline{G}_{n-k}, t_{n-k}) + 90\sum_{k=1}^{n-1}(n-k+1) - 63(n-1) \\ &= 27 + 6\sum_{k=1}^{n-1} W(\overline{G}_k, t_k) + 45(n+2)(n-1) - 63(n-1) \\ &= 6\sum_{k=1}^{n-1} W(\overline{G}_k, t_k) + 45n^2 - 18n, \end{aligned}$$

i.e.,

$$W(\overline{G}_n) = 6\sum_{k=1}^{n-1} W(\overline{G}_k, t_k) + 45n^2 - 18n. \tag{8}$$

And,

$$\begin{aligned} W(\overline{G}_k, t_k) &= W(\overline{G}_{k-1}, t_{k-1}) + g(t_k) \\ &= W(\overline{G}_1, t_1) + g(t_2) + \cdots + g(t_k) \\ &= g(t_1) + g(t_2) + \cdots + g(t_k), \end{aligned}$$

i.e.,

$$W(\overline{G}_k, t_k) = \sum_{i=1}^{k} g(t_i). \tag{9}$$

Combining equations (8) and (9), we can obtain the following formula for computing the Wiener indices of polyphenyl hexagonal chains.

Theorem 3.2. Let $\overline{G}_n = \overline{H}_0\overline{H}_1 \cdots \overline{H}_{n-1}$ be a polyphenyl hexagonal chain with n hexagons, t_k the tail of $\overline{H}_k$, $1 \leq k \leq n-1$. Then

$$\begin{aligned} W(\overline{G}_n) &= 6\sum_{k=1}^{n-1}\sum_{i=1}^{k} g(t_i) + 45n^2 - 18n \\ &= 6\sum_{k=1}^{n-1}(n-k)g(t_k) + 45n^2 - 18n, \end{aligned}$$

where

$$g(t_k) = \begin{cases} 12(k-1)+9, & t_k \ is \ o_{k-1}; \\ 18(k-1)+9, & t_k \ is \ m_{k-1}; \\ 24(k-1)+9, & t_k \ is \ p_{k-1}. \end{cases} \tag{10}$$

and $g(t_1) = 9$.

For the polyphenyl orth-chain $\overline{O}_n$, the polyphenyl meta-chain $\overline{M}_n$ and the polyphenyl para-chain $\overline{L}_n$, t_k is o_{k-1}, m_{k-1} and p_{k-1}, respectively. So, we have

$W(\overline{O}_n) = 6\sum_{k=1}^{n-1}(n-k)(12(k-1)+9) + 45n^2 - 18n = 12n^3 + 36n^2 - 21n;$

$W(\overline{M}_n) = 6\sum_{k=1}^{n-1}(n-k)(15(k-1)+9) + 45n^2 - 18n = 18n^3 + 18n^2 - 9n;$

$W(\overline{P}_n) = 6\sum_{k=1}^{n-1}(n-k)(24(k-1)+9) + 45n^2 - 18n = 24n^3 + 3n.$

Corollary 3.3. The Wiener indices of the polyphenyl orth-chain $\overline{O}_n$, the polyphenyl meta-chain $\overline{M}_n$ and the polyphenyl para-chain $\overline{L}_n$ are

$$W(\overline{O}_n) = 12n^3 + 36n^2 - 21n;$$

$$W(\overline{M}_n) = 18n^3 + 18n^2 - 9n;$$

$$W(\overline{P}_n) = 24n^3 + 3n.$$

4 A relation between $W(G_n)$ and $W(\overline{G}_n)$

An exact relation between the Wiener indices of a phenylene and its hexagonal squeeze was established by Pavlović and Gutman [13].

To every polyhenyl hexagonal chain, it is possible to associate a spiro hexagonal chain, obtained so that the cut edges of the polyphenyl hexagonal chain are squeezed off. This spiro hexagonal chain is named the hexagonal squeeze of the respective polyphenyl hexagonal chain. Clearly, each polyhenyl hexagonal chain determines a unique hexagonal squeeze and vice versa, and these two systems have an equal number of hexagons. For example, the spiro hexagonal chain in Figure 2(i) is the hexagonal squeeze of the polyphenyl hexagonal chain in Figure 2(ii). Here, we also give a relation between the Wiener indices of a polyphenyl hexagonal chain and its hexagonal squeeze.

Theorem 4.1. Let $\overline{G}_n = \overline{H}_0\overline{H}_1 \cdots \overline{H}_{n-1}$ be a polyphenyl hexagonal chain with n hexagons, $G_n = H_0H_1 \cdots H_{n-1}$ its hexagonal squeeze. The Wiener indices of $\overline{G}_n$ and G_n are related as

$$25W(\overline{G}_n) = 36W(G_n) + 150n^3 - 270n^2 - 177n. \tag{11}$$

Proof. From equations (5) and (10), we have

$$\frac{g(t_k) - 9}{6} = \frac{f(c_k) - 9}{5} + (k-1),$$

i.e.,

$$5g(t_k) = 6f(c_k) + 30k - 39.$$

So,

$$5\sum_{k=1}^{n-1}(n-k)g(t_k) = 6\sum_{k=1}^{n-1}(n-k)f(c_k) + \sum_{k=1}^{n-1}(n-k)(30k-39).$$

By Theorems 2.2 and 3.2,

$$\frac{5}{6}W(\overline{G}_n) - \frac{5}{6}(45n^2 - 18n) = \frac{6}{5}W(G_n) - \frac{6}{10}(45n^2 + 9n) + \sum_{k=1}^{n-1}(n-k)(30k-39),$$

i.e.,

$$\frac{5}{6}W(\overline{G}_n) = \frac{6}{5}W(G_n) + 5n^3 - 9n^2 - \frac{59}{10}n$$

and

$$25W(\overline{G}_n) = 36W(G_n) + 150n^3 - 270n^2 - 177n.$$

From Theorem 4.1, we can obtain the following result on the extremal problems of polyphenyl hexagonal chains with respect to the Wiener index.

Theorem 4.2. (i) Among all polyphenyl hexagonal chains with $n(n \geq 4)$ hexagons, $\overline{G}_n$ has the minimum, the second and the third minimal Wiener index if and only if its hexagonal squeeze G_n has the minimum, the second and the third minimal Wiener index among all spiro hexagonal chains with n hexagons.

(ii) Among all polyphenyl hexagonal chains with $n(n \geq 4)$ hexagons, $\overline{G}_n$ has the maximum, the second and the third maximal Wiener index if and only if its hexagonal squeeze G_n has the maximum, the second and the third maximal Wiener index among all spiro hexagonal chains with n hexagons.

5 The average value of the Wiener index

If $\mathcal{G}_n$ is the set of all spiro hexagonal chains with n hexagons, then the average value of the Wiener indices with respect to $\mathcal{G}_n$ is

$$W_{avr}(\mathcal{G}_n) = \frac{1}{|\mathcal{G}_n|} \sum_{G \in \mathcal{G}_n} W(G).$$

Let $G_n = H_0 H_1 \cdots H_{n-1}$ be a spiro hexagonal chain of length n. c_k is the common cut-vertex of H_{k-1} and H_k, $k = 1, 2, \cdots, n-1$. H_k is called ortho-hexagon, meta-hexagon, or para-hexagon in [9] if the distance between its cut-vertices c_{k-1} and c_k is 1, 2, and 3, respectively. In an obvious way, each spiro hexagonal chain of length n can be assigned a word of length $n-2$ over the alphabet $\{O, M, P\}$. Such a word is called the code of the chain. For example, the code of the chain in Figure 3(i) is PMMMO. The correspondence is not necessarily bijective: the same chain is also described by the code OMMMP, i.e., the same code read backwards. It is easy to see that a palindromic code uniquely defines a chain, while exactly two non-palindromic

codes correspond to the same chain. From here, it was concluded in [9] that the number of all possible spiro hexagonal chains of length n is equal to the number obtained by adding half the number of non-palindromic codes of length $n-2$ to the number of palindromic codes of the same length. Since the number of palindromic codes of length n is equal to $3^{\lfloor\frac{n+1}{2}\rfloor}$ and the total number of codes is equal to 3^n, we have the following result.

Lemma 5.1([9]). The number of different spiro hexagonal chains of length n is

$$|\mathcal{G}_n| = \frac{1}{2}(3^{n-2} + 3^{\lfloor\frac{n-1}{2}\rfloor}).$$

Since $f(c_1) = 9$, from Theorem 2.2, the Wiener index of a spiro hexagonal chain G_n of length n can be reduced to

$$W(G_n) \quad = 5\sum_{k=2}^{n-1}(n-k)f(c_k) + \tfrac{9}{2}(5n^2 + 11n - 10).$$

Let $G_n = H_0H_1\cdots H_{n-1}$ be a spiro hexagonal chain of length n. $x_1x_2\cdots x_{n-2}$ is its code, where $x_i \in \{O, M, P\}$. $(c_2, c_3, \cdots, c_{n-1})$ is its cut-vertex sequence. Then

$$\begin{cases} x_i = O & \text{if and only if} \quad c_{i+1} = o_i; \\ x_i = M & \text{if and only if} \quad c_{i+1} = m_i; \\ x_i = P & \text{if and only if} \quad c_{i+1} = p_i. \end{cases}$$

Note that each of $o_{k-1}, m_{k-1}, p_{k-1}$ can be taken 3^{n-3} times by c_k when $(c_2, \cdots, c_{n-1})$ is taken over all the sequences of length $n-2$, and each of $o_{k-1}, m_{k-1}, p_{k-1}$ can be taken by $3^{\lfloor\frac{n-3}{2}\rfloor}$ times c_k when $(c_2, \cdots, c_{n-1})$ is taken over all the palindromic sequences of length $n-2$. We have the following result

$$\sum_{G_n\in\mathcal{G}_n} W(G_n) = \tfrac{1}{2}(\textstyle\sum_1 W(G_n) + \sum_2 W(G_n))$$

where $\sum_1$ is taken over all G_n whose cut-vertex sequences $(c_2, \cdots, c_{n-1})$ are the sequences of length $n-2$, and $\sum_2$ is taken over all G_n whose cut-vertex sequences $(c_2, \cdots, c_{n-1})$ are the palindromic sequences of length $n-2$. So,

$$\begin{aligned} \textstyle\sum_1 W(G_n) \quad &= \quad 3^{n-3} \times 5\sum_{k=2}^{n-1}(n-k)[f(o_{k-1}) + f(m_{k-1}) + f(p_{k-1})] \\ &\quad\quad +\tfrac{9}{2}(5n^2 + 11n - 10) \times 3^{n-2} \\ &= \quad 3^{n-3} \times 5\sum_{k=2}^{n-1}(n-k)[30(k-1) + 27] + \tfrac{3^n}{2}(5n^2 + 11n - 10) \\ &= \quad 3^{n-3} \times 5 \times (5n^3 - \tfrac{3}{2}n^2 - \tfrac{61}{2}n + 27) + \tfrac{3^n}{2}(5n^2 + 11n - 10) \\ &= \quad 3^{n-3}(25n^3 + 60n^2 - 4n) \end{aligned}$$

$$\begin{aligned}\textstyle\sum_2 W(G_n) &= 3^{\lfloor\frac{n-3}{2}\rfloor}\times 5\sum_{k=2}^{n-1}(n-k)[f(o_{k-1})+f(m_{k-1})+f(p_{k-1})] \\ &\quad +\tfrac{9}{2}(5n^2+11n-10)\times 3^{\lfloor\frac{n-1}{2}\rfloor} \\ &= 3^{\lfloor\frac{n-3}{2}\rfloor}(25n^3+60n^2-4n)\end{aligned}$$

and

$$\sum_{G_n\in\mathcal{G}_n} W(G_n)=\frac{1}{2}(3^{n-3}+3^{\lfloor\frac{n-3}{2}\rfloor})(25n^3+60n^2-4n).$$

By Lemma 5.1, we can get the average value of the Wiener indices with respect to $\mathcal{G}_n$.

Theorem 5.2. The average value of the Wiener indices with respect to $\mathcal{G}_n$ is

$$W_{avr}(\mathcal{G}_n)=\frac{1}{3}(25n^3+60n^2-4n).$$

Note that the average value of the Wiener indices with respect to $\{O_n, M_n, P_n\}$ is

$$\frac{W(O_n)+W(M_n)+W(P_n)}{3}=\frac{1}{3}(25n^3+60n^2-4n)$$

from Corollary 2.3. The interesting result shows that the average value of the Wiener indices with respect to $\mathcal{G}_n$ is exactly the average value of the Wiener indices with respect to $\{O_n, M_n, P_n\}$, and is just the Wiener index $W(M_n)$ of the spiro meta-chain M_n.

Similarly, if $\overline{\mathcal{G}}_n$ is the set of all polyphenyl hexagonal chains with n hexagons, then the average value of the Wiener indices with respect to $\overline{\mathcal{G}}_n$ is

$$W_{avr}(\overline{\mathcal{G}}_n)=\frac{1}{|\overline{\mathcal{G}}_n|}\sum_{G\in\overline{\mathcal{G}}_n} W(G).$$

Using the hexagonal squeeze, there is a bijection between $\overline{\mathcal{G}}_n$ and $\mathcal{G}_n$. So, we have

$$|\overline{\mathcal{G}}_n|=|\mathcal{G}_n|=\frac{1}{2}(3^{n-2}+3^{\lfloor\frac{n-1}{2}\rfloor})$$

and

$$\sum_{\overline{G}_n\in\overline{\mathcal{G}}_n} W(\overline{G}_n)=\tfrac{1}{2}(\textstyle\sum_1 W(\overline{G}_n)+\sum_2 W(\overline{G}_n))$$

where $\sum_1$ is taken over all $\overline{G}_n$ whose cut-vertex sequences $(c_2,\cdots,c_{n-1})$ of their hexagonal squeezes are the sequences of length $n-2$, and $\sum_2$ is taken over all $\overline{G}_n$ whose

cut-vertex sequences $(c_2, \cdots, c_{n-1})$ of their hexagonal squeezes are the palindromic sequences of length $n-2$.

Since $g(t_1) = 9$, from Theorem 3.2, the Wiener index of a polyphenyl hexagonal chain $\overline{G}_n$ of length n can be reduced to

$$W(\overline{G}_n) \;= 6\sum_{k=2}^{n-1}(n-k)g(t_k) + (45n^2 + 36n - 54).$$

$$\begin{aligned}
\textstyle\sum_1 W(\overline{G}_n) &= 3^{n-3} \times 6\sum_{k=2}^{n-1}(n-k)[g(o_{k-1}) + g(m_{k-1}) + g(p_{k-1})] \\
&\quad +3^{n-2}(45n^2 + 36n - 54) \\
&= 3^{n-3} \times 6\sum_{k=2}^{n-1}(n-k)[54(k-1) + 27] + 3^{n-2}(45n^2 + 36n - 54) \\
&= 3^{n-3}(54n^3 - 81n^2 - 135n + 162) + 3^{n-2}(45n^2 + 36n - 54) \\
&= 3^{n-3}(54n^3 + 54n^2 - 27n)
\end{aligned}$$

$$\begin{aligned}
\textstyle\sum_2 W(\overline{G}_n) &= 3^{\lfloor\frac{n-3}{2}\rfloor} \times 6\sum_{k=2}^{n-1}(n-k)[g(o_{k-1}) + g(m_{k-1}) + g(p_{k-1})] \\
&\quad +3^{\lfloor\frac{n-1}{2}\rfloor}(45n^2 + 36n - 54) \\
&= 3^{\lfloor\frac{n-3}{2}\rfloor}(54n^3 + 54n^2 - 27n)
\end{aligned}$$

and

$$\sum_{\overline{G}_n \in \mathcal{G}_n} W(G_n) = \frac{1}{2}(3^{n-3} + 3^{\lfloor\frac{n-3}{2}\rfloor})(54n^3 + 54n^2 - 27n).$$

Hence, we can get the average value of the Wiener indices with respect to $\overline{\mathcal{G}}_n$.

Theorem 5.3. The average value of the Wiener indices with respect to $\overline{\mathcal{G}}_n$ is

$$W_{avr}(\overline{\mathcal{G}}_n) = 18n^3 + 18n^2 - 9n.$$

Note that the average value of the Wiener indices with respect to $\{\overline{O}_n, \overline{M}_n, \overline{P}_n\}$ is

$$\frac{W(\overline{O}_n) + W(\overline{M}_n) + W(\overline{P}_n)}{3} = 18n^3 + 18n^2 - 9n$$

from Corollary 3.3. This also shows that the average value of the Wiener indices with respect to $\overline{\mathcal{G}}_n$ is exactly that to $\{\overline{O}_n, \overline{M}_n, \overline{P}_n\}$, and is just the Wiener index of the polyphenyl meta-chain $\overline{M}_n$.

Finally, by Theorems 5.2 and 5.3, we have

$$25W_{avr}(\overline{\mathcal{G}}_n) = 36W_{avr}(\mathcal{G}_n) + 150n^3 - 270n^2 - 177n.$$

This relation is identical with the equation (11) in Theorem 4.1.

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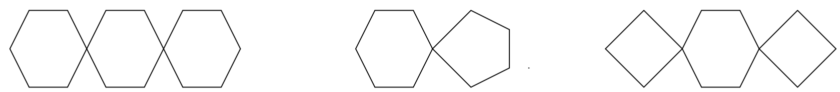
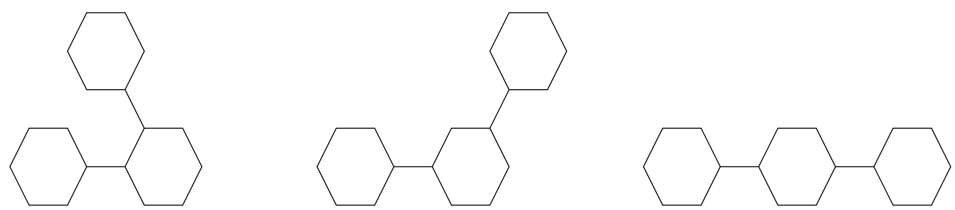
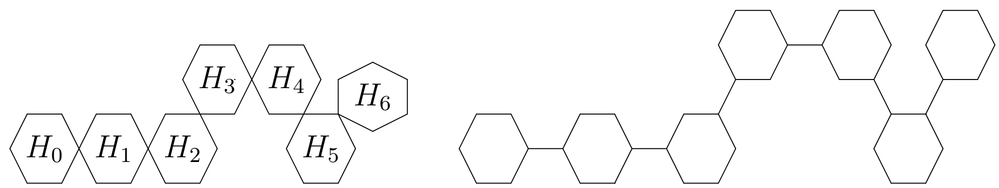


(i) dispiro[5,2,5]hexadecane spiro[4,5]decane dispiro[3,2,3,2]dodecane



(ii) ortho-terphenyl meta-terphenyl pera-terphenyl

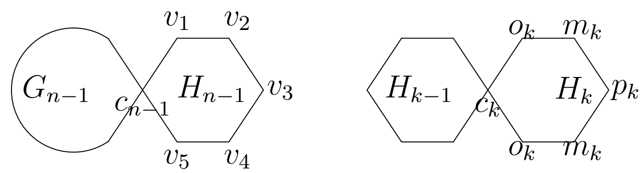
Figure 1. (i) Three linear polyspiro alicyclic hydrocarbons.
(ii) Ortho-terphenyl, meta-terphenyl and pera-terphenyl.



(i) A spiro hexagonal chain of length 7 with the cut-vertex sequence $(p_1, m_2, m_3, m_4, o_5)$.

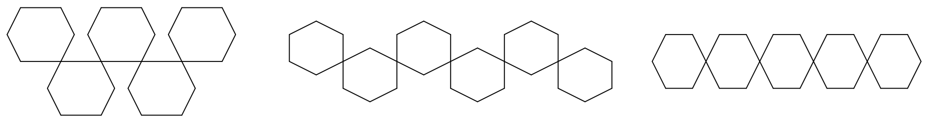
(ii) A polyphenyl hexagonal chain of length 7.

Figure 2. A spiro hexagonal chain and a polyphenyl hexagonal chain.



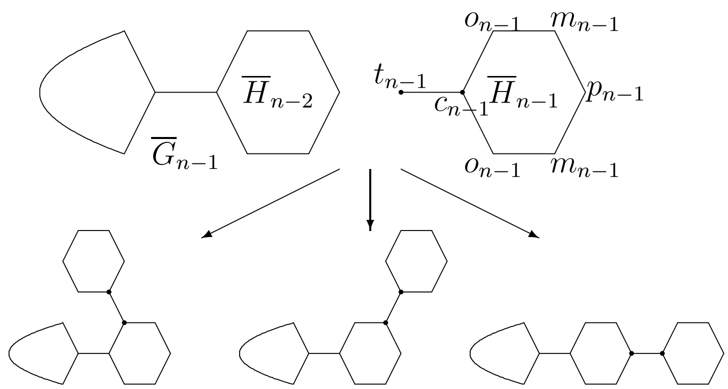
(i) G_n (ii)

Figure 3. Ortho-, meta-, and para-vertices.



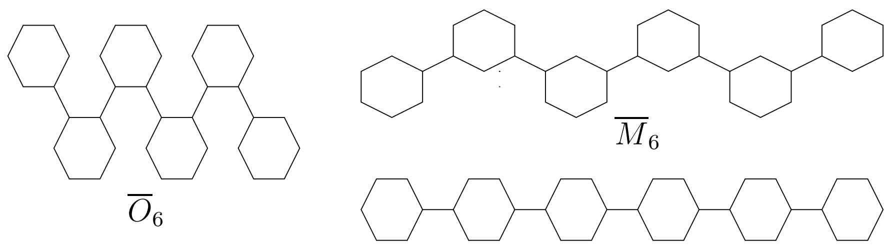
O_5 M_6 P_5

Figure 4.



o_{n-1}
m_{n-1}
t_{n-1}
$\overline{H}_{n-2}$
c_{n-1}
$\overline{H}_{n-1}$
p_{n-1}
$\overline{G}_{n-1}$
o_{n-1}
m_{n-1}

Figure 5.



$\overline{O}_6$ $\overline{M}_6$ $\overline{P}_6$

Figure 6.